

wwPDB X-ray Structure Validation Summary Report (i)

Oct 19, 2023 – 12:22 PM JST

:	8JZH
:	C. glutamicum S-adenosylmethionine synthase
:	Lee, S.; Kim, K.J.
	2023-07-05
:	2.20 Å(reported)
	:

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

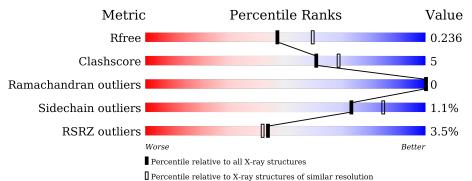
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
1	А	412	^{2%} 86%	8%	6%
1	В	412	87%	7%	• 6%
1	С	412	6% 81%	13%	6%



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9681 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	389	Total	С	Ν	Ο	\mathbf{S}	0	Ο	0
	Π	369	2977	1867	521	582	7	0	0	0
1	В	389	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	D	569	2989	1874	526	582	7	0		
1	С	386	Total	С	Ν	Ο	S	0	0	0
	I C		2958	1852	519	580	7	0	0	0

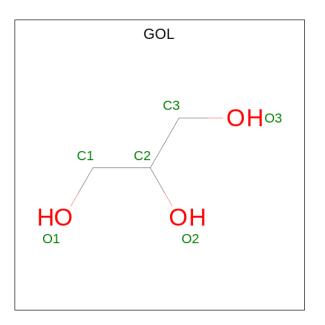
• Molecule 1 is a protein called S-adenosylmethionine synthase.

Chain	Residue	Modelled	Actual	Comment	Reference
А	408	LEU	-	expression tag	UNP Q9K5E4
А	409	GLU	-	expression tag	UNP Q9K5E4
А	410	HIS	-	expression tag	UNP Q9K5E4
А	411	HIS	-	expression tag	UNP Q9K5E4
А	412	HIS	-	expression tag	UNP Q9K5E4
В	408	LEU	-	expression tag	UNP Q9K5E4
В	409	GLU	-	expression tag	UNP Q9K5E4
В	410	HIS	-	expression tag	UNP Q9K5E4
В	411	HIS	-	expression tag	UNP Q9K5E4
В	412	HIS	-	expression tag	UNP Q9K5E4
С	408	LEU	-	expression tag	UNP Q9K5E4
С	409	GLU	-	expression tag	UNP Q9K5E4
С	410	HIS	-	expression tag	UNP Q9K5E4
С	411	HIS	-	expression tag	UNP Q9K5E4
С	412	HIS	-	expression tag	UNP Q9K5E4

There are 15 discrepancies between the modelled and reference sequences:

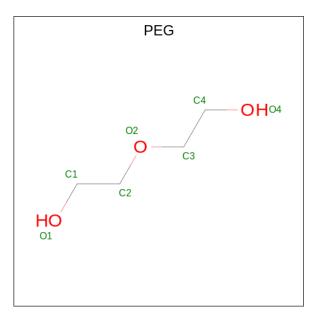
• Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	А	1	Total 7	C 4	0 3	0	0

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BANK

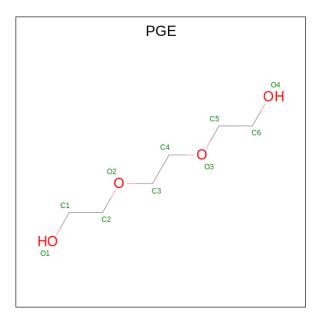
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0

• Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mo	l Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Na 1 1	0	0
4	В	2	Total Na 2 2	0	0

• Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	В	1	Total 10	C 6	0 4	0	0

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N	Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
	5	С	1	Total 10	С 6	0 4	0	0

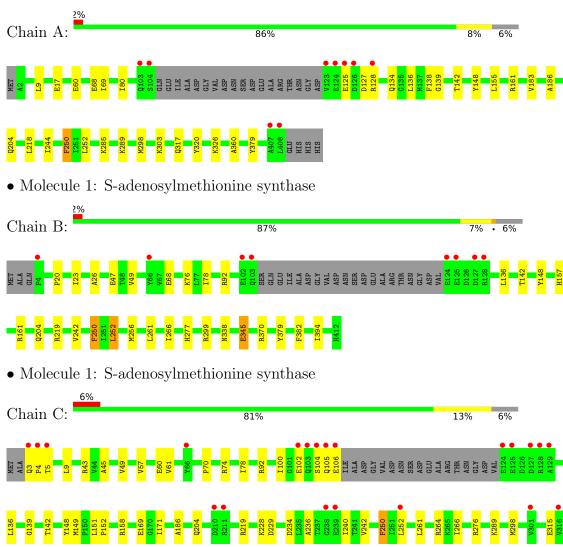
• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	263	Total O 263 263	0	0
6	В	192	Total O 192 192	0	0
6	С	212	Total O 212 212	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: S-adenosylmethionine synthase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants	129.15Å 203.89Å 144.19Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.48 - 2.20	Depositor
Resolution (A)	29.47 - 2.20	EDS
% Data completeness	98.6 (29.48-2.20)	Depositor
(in resolution range)	98.7 (29.47-2.20)	EDS
R _{merge}	0.08	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$5.77 (at 2.20 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
D D	0.183 , 0.229	Depositor
R, R_{free}	0.197 , 0.236	DCC
R_{free} test set	4851 reflections $(5.08%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	36.6	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34,40.8	EDS
L-test for twinning ²	$ L > = 0.52, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9681	wwPDB-VP
Average B, all atoms $(Å^2)$	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NA, PEG, PGE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Boi	nd lengths	Bond angles	
IVIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.70	1/3029~(0.0%)	0.77	0/4116
1	В	0.74	0/3044	0.91	2/4135~(0.0%)
1	С	0.60	0/3010	0.68	0/4089
All	All	0.68	1/9083~(0.0%)	0.79	2/12340~(0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	60	GLU	CD-OE1	6.01	1.32	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	370	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	В	370	ARG	NE-CZ-NH2	-5.70	117.45	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2977	0	2948	21	0
1	В	2989	0	2949	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes		
1	С	2958	0	2917	39	0		
2	А	12	0	16	1	0		
2	В	6	0	8	0	0		
3	А	35	0	50	6	0		
3	В	14	0	20	0	0		
4	А	1	0	0	0	0		
4	В	2	0	0	0	0		
5	В	10	0	14	0	0		
5	С	10	0	14	3	0		
6	А	263	0	0	2	0		
6	В	192	0	0	3	0		
6	С	212	0	0	0	0		
All	All	9681	0	8936	81	0		

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The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 81 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:VAL:HG21	1:C:49:VAL:HG21	1.50	0.93
1:A:303:LYS:HZ1	3:A:505:PEG:H31	1.35	0.92
1:B:345:GLU:OE2	6:B:601:HOH:O	1.93	0.84
1:C:326:LYS:HD2	1:C:327:PRO:HD2	1.71	0.70
1:B:161:ARG:HH11	1:B:379:TYR:HB3	1.55	0.70

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	385/412~(93%)	376~(98%)	9~(2%)	0	100	100
1	В	385/412~(93%)	373~(97%)	12 (3%)	0	100	100
1	С	382/412~(93%)	369~(97%)	13 (3%)	0	100	100
All	All	1152/1236~(93%)	1118 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	314/333~(94%)	310~(99%)	4 (1%)	69 81
1	В	315/333~(95%)	311~(99%)	4 (1%)	69 81
1	С	312/333~(94%)	310~(99%)	2(1%)	86 93
All	All	941/999~(94%)	931 (99%)	10 (1%)	73 85

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	345	GLU
1	С	136	LEU
1	С	250	PHE
1	А	326	LYS
1	В	136	LEU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such side chains are listed below:

Mol	Chain	Res	Type
1	С	71	GLN
1	С	190	GLN
1	С	221	HIS



5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Mol Type Chain		Res Link		B	Bond lengths			Bond angles		
	Type	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
2	GOL	В	503	-	$5,\!5,\!5$	0.12	0	$5,\!5,\!5$	0.57	0	
2	GOL	А	502	-	$5,\!5,\!5$	0.08	0	$5,\!5,\!5$	0.35	0	
3	PEG	А	506	-	6,6,6	0.19	0	$5,\!5,\!5$	0.27	0	
5	PGE	С	501	-	9,9,9	0.35	0	8,8,8	0.56	0	
3	PEG	А	503	-	6,6,6	0.48	0	$5,\!5,\!5$	0.20	0	
5	PGE	В	501	-	9,9,9	0.28	0	8,8,8	0.12	0	
3	PEG	В	502	-	6,6,6	0.24	0	$5,\!5,\!5$	0.20	0	
3	PEG	А	504	-	6,6,6	0.33	0	$5,\!5,\!5$	0.24	0	
3	PEG	В	504	-	6,6,6	0.48	0	$5,\!5,\!5$	0.39	0	
3	PEG	А	505	-	6,6,6	0.32	0	$5,\!5,\!5$	0.30	0	
3	PEG	А	507	-	6,6,6	0.56	0	$5,\!5,\!5$	0.58	0	
2	GOL	А	501	-	$5,\!5,\!5$	0.17	0	$5,\!5,\!5$	0.35	0	

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	В	503	-	-	1/4/4/4	-
2	GOL	А	502	-	-	1/4/4/4	-
3	PEG	А	506	-	-	3/4/4/4	-
5	PGE	С	501	-	-	3/7/7/7	-
3	PEG	А	503	-	-	1/4/4/4	-
5	PGE	В	501	-	-	5/7/7/7	-
3	PEG	В	502	-	-	1/4/4/4	-
3	PEG	А	504	-	-	3/4/4/4	-
3	PEG	В	504	-	-	2/4/4/4	-
3	PEG	А	505	-	-	2/4/4/4	-
3	PEG	А	507	-	-	2/4/4/4	-
2	GOL	А	501	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	501	GOL	O1-C1-C2-C3
3	А	505	PEG	O1-C1-C2-O2
3	А	507	PEG	O2-C3-C4-O4
5	В	501	PGE	O1-C1-C2-O2
3	А	504	PEG	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	502	GOL	1	0
3	А	506	PEG	2	0
5	С	501	PGE	3	0
3	А	505	PEG	3	0
3	А	507	PEG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.



5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$\langle RSRZ \rangle$	# RSRZ > 2	$OWAB(Å^2)$	$\mathbf{Q} {<} 0.9$
1	А	389/412~(94%)	-0.25	9 (2%) 60 58	24, 34, 60, 156	0
1	В	389/412~(94%)	-0.22	8 (2%) 63 61	28, 39, 67, 115	0
1	С	386/412~(93%)	-0.09	24 (6%) 20 19	28, 39, 71, 125	0
All	All	1164/1236~(94%)	-0.19	41 (3%) 44 42	24, 38, 68, 156	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	123	VAL	9.0
1	С	128	ARG	7.1
1	А	125	GLU	7.0
1	А	124	GLU	6.6
1	В	124	GLU	5.9

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
3	PEG	В	504	7/7	0.71	0.29	74,80,84,94	0
3	PEG	А	505	7/7	0.72	0.17	69,73,78,87	0
3	PEG	А	506	7/7	0.76	0.23	61,73,86,87	0
3	PEG	А	503	7/7	0.77	0.16	58,71,77,82	0
4	NA	В	505	1/1	0.77	0.18	29,29,29,29	0
5	PGE	В	501	10/10	0.77	0.21	70,81,84,86	0
3	PEG	А	507	7/7	0.79	0.19	43,53,57,59	0
3	PEG	А	504	7/7	0.79	0.17	50,58,63,64	0
4	NA	В	506	1/1	0.82	0.21	32,32,32,32	0
2	GOL	В	503	6/6	0.85	0.18	48,59,61,68	0
2	GOL	А	502	6/6	0.85	0.18	$38,\!42,\!52,\!57$	0
4	NA	А	508	1/1	0.90	0.23	$25,\!25,\!25,\!25$	0
3	PEG	В	502	7/7	0.91	0.12	53,55,61,62	0
2	GOL	А	501	6/6	0.91	0.08	40,51,54,55	0
5	PGE	С	501	10/10	0.91	0.13	43,50,61,65	0

6.5 Other polymers (i)

There are no such residues in this entry.

